Laboratory Name: Oak Ridge National Laboratory
B&R Code: KC 0203010

FWP and possible subtask under FWP:
Chemistry of Advanced Inorganic Materials

FWP Number: ERKCC01

Program Scope: The goal of this program is to develop and advance methods for the synthesis, characterization and manipulation of novel materials. Materials currently under investigation include metal and metal oxide nanoparticles, thin-film ceramics including cuprate superconductors, buffer layers for high-current superconducting films, and optoelectronic materials. Methods of synthesis include wet chemical synthesis of nanoparticles in micelle reactors, sol-gel synthesis of thin films, and vacuum techniques for the synthesis of metallic and metal oxide nanocrystals. Techniques for materials characterization include surface probe and electron microscopy, X-ray/neutron diffraction (NXRD), inelastic neutron scattering (INS), and various thermodynamic techniques. These techniques are used to develop a quantitative, molecular level description of molecule-molecule and molecule-surface interactions by collecting detailed information regarding structure, dynamics and chemical activity.

Major Program Achievements (over duration of support):
-Studies of self-assembly phenomena in nanoscale space confined environments revealed a "critical diameter" of pore channels (around 50 nm), below which homogeneous mesophase forms. However, above such critical diameter, mixed phases (amorphous, hexagonal, lamellar) exist.
- Inelastic study of Bose-Einstein condensates of liquid ^{4}He near an MgO surface showed evidence for a BE condensate in surface films and an increase in the kinetic energy of ^{4}He atoms as film thickness is reduced.
-General synthetic method for the synthesis of 2 nm diameter oxide ferroelectric nanoparticles was developed.

Program impact: The efforts of this program will have significant impact in the areas of nanoscience and technology, electrical power transmission and utilization, microelectronics, chemical sensors, lubrication, catalysis and environmentally relevant materials.

Interactions:
Los Alamos National Lab LANSCE (L. Daemen)
Cambridge University (S. Clarke, A. Alavi, R. Lynden-Bell)
Institute Laue Langevin (J. Pierce, M. Gonzalez, T. Hansen, T. Seydal)
University of Madrid (D. Martin y Marrero)
Tennessee Technological University (John Zhu)
University of Tennessee (N. Dahotre)
University of Maryland (M. Harris)
Rutherford Appleton Lab ISIS (A. Ramirez-Cuesta, S.Parker, J. Tomkinson)
University of Delaware (H. Glyde)
University of Tennessee (R. Hinde)
University of Tennessee (Z. Xue)
University of Cincinnati (D.L. Shi)
University of Washington (G.Z. Cao)
University of Akron (Y. Qiao)
American Superconductor Inc. (M. Rupich)

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
-Editorial Board Member, Superconductor Science and Technology; Associate Editor, Journal of the American Ceramic Society (M. Paranthaman)
- Editor-in-Chief for Journal of Nanomaterials (M. Hu)
-Team Leader/spokesperson, ***VISION*** neutron vibrational spectrometer for the SNS (Larese)
-Wigner Fellow (A. Rondinone)

Personnel Commitments for FY2005 to Nearest +/- 10%:
D. B. Beach (group leader) 50%
J. Z. Larese (ORNL/UTK joint facility appointment) 60%
A. J. Rondinone (ORNL staff scientist) 20%
M. Z. Hu (ORNL staff scientist) 50%
M. Paranthaman (ORNL staff scientist) 20%
Z. Pan (ORNL staff scientist) 20%
R. Cook, M. Farianelli, L. Frasier, G. Thomas (UTK students at ORNL) 50%

Authorized Budget (BA) for FY03, FY04, FY05:
FY03 BA $430,000 **FY04 BA** $895,000 **FY05 BA** $990,000

Laboratory Name: Oak Ridge National Lab
B&R Code: KC 02 03 01

FWP and possible subtask under FWP:
Polymer-based Multicomponent Materials

FWP Number: ERKCC02

Program Scope: Combining experimental, theoretical and synthetic approaches, we perform fundamental studies of the structure, dynamics and thermodynamics of macromolecular systems to provide a better understanding of the macroscopic properties of advanced polymeric materials. Major experimental tools include a full suite of synthetic methods, including anionic polymerization, X-ray and neutron scattering methods, NMR and neutron spectroscopy, atomic probe and optical microscopies, and state-of-the-art thermal analysis, including temperature modulated DSC and AFM-based microcalorimetry. Simulation and theoretical approaches include molecular dynamics, Monte Carlo, mean field, lattice, and integral equation theory.

Major Program Achievements (over duration of support): The structure of polymer-nanoparticle mixtures have been examined through novel syntheses and theoretical methods. Poly(styrene)-like, crosslinked nanoparticles have been synthesized with controllable particle size, softness and surface decoration. The effect of chemically-controllable polymer-nanoparticle attractive interactions on the structure and thermodynamics of polymer nanocomposites were obtained from PRISM theory. A *priori* prediction of the strength of multigraft polymers as a function of the number and types of grafts from large-scale atomistic Monte Carlo, molecular mechanics, and molecular dynamics simulations were developed. Several triblock copolymers likely to form triply periodic and multiply continuous network phases were synthesized, and their phase behavior was investigated using small-angle x-ray scattering, dynamic mechanical spectroscopy, and electron microscopy. Conformational changes of stretched rubbery polymers are studied using Raman and inelastic neutron scattering. The structure and thermodynamic properties of poly(alkylsiloxanes), poly(styrene), isotactic poly(propylene), poly(ethylene/ethylethylene) and their blends and copolymers were examined using wide-angle X-ray and small angle neutron scattering, and PRISM integral equation theory. A thermodynamic description of partially crystalline, linear macromolecules has been developed as a macroscopic, globally metastable structure which consists of multiple nanophases.

Program impact: Provides insights on the microscopic origins of macroscopic properties of polymer solids, melts, blends, alloys and composites, co-polymers, micellar systems, and small molecule analogs. Investigators include world leaders in the physics, chemistry and synthesis of polymers, the structure, dynamics and advanced thermal analysis, and the statistical mechanics and simulation of macromolecular systems.

Interactions: National Laboratories: ORNL, ANL, LANL, LLNL, NIST, Sandia; National and international user facilities: CNMS, HFIR, IPNS, APS, NCNR, LANSCE, ISIS, Risø, Forschungszentrum (Juelich), Saclay; Universities: collaborations/interactions with over fifty US and foreign universities; Industry: Dow, Schlumberger, Medtronic, PolyE, 3M, Fleetguard, ChevronPhillips, Rhodia, Goodyear, Mitsubishi, Dow, National Starch, Avanti Polar Lipids, Du Pont, Roehm GmbH, Shell, Dow-Cargill, Metabolix.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
Five APS and one NATAS Fellows; one National Academy of Engineering member; MRS David Turnbull Lectureship Award; APS High Polymer Physics Prize winner; two APS Dillon Medals; former president, Neutron Scattering Society of America, three Distinguished Scientists/Professors; two Chairs of APS Polymer Physics Division; DOE-BES Award for Outstanding Scientific Accomplishment in Materials Chemistry; an R&D100 Award; Presidential Green Chemistry Challenge Award; Paul W. Schmidt Memorial Award; Arnold Beckman Award; two ACS Doolittle Awards, and many other awards; numerous regional, national, and international and DOE advisory committee members; twenty journal editorial/advisory boards; ~140 refereed papers in last 3 years.

Personnel Commitments for FY2005 to Nearest +/- 10%:
A. Habenschuss (60%), B. K. Annis (70%), V. Urban (10%), B. Wunderlich (emeritus, 0%), J. W. Mays (ORNL/U. Tenn. Distinguished Scientist, 50%), M. D. Dadmun (ORNL/U. Tenn., 25%), D. W. Noid (20%), B. G. Sumpter (40%), G. D. Wignall (10%), J. G. Curro, (Sandia, 25%), K. S. Schweizer (U. Ill, 33%), F. S. Bates (U. Minn., 33%), Pradeep Kumar (postdoc, 100%)

Authorized Budget (BA) for FY03, FY04, FY05:
FY03 BA $1,760K FY04 BA $1,465K FY05 BA $1,785K

Laboratory Name: Oak Ridge National Laboratory
B&R Code: KC 02 01 01 0 & KC 02 06 01 0

FWP: Theoretical Studies of Metals, Alloys, and Ceramics

FWP Number: ERKCM01

Program Scope: First-principles theory is used to predict materials properties, relate them to the electronic structure, provide fundamental insights, and guide experimental programs in alloy and ceramic development and nanoscience. Molecular dynamics, based on first principles derived potentials, is used to study the influence of nanoscale defects on macroscopic properties. Global optimization and parallel algorithms are used to extend the applicability of first-principles approaches to experimentally relevant nanostructures.

Major Program Achievements (over duration of support): Pioneered the development of a number of first principles electronic structure methods and their use in guiding alloy and ceramic development including: the KKR-CPA theory of the electronic structure and phase stability of alloys; the self-consistent partial-wave (SCPW) cluster technique and its use in the study of intergranular films and rare earth dopants in ceramics; highly accurate full potential linearized augmented plane wave (FLAPW) calculations of the properties of intermetallic compounds to predict mechanical behavior; the parallel LSMS method and spin dynamics calculations of the magnetic structure of alloys and nanostructures. We have developed a first principles differential binding energy model to predict the effects of dopants on grain growth. First-principles methods have also been used to determine helium defect properties in BCC transition metal hosts, and to study the properties of experimentally realizable nanostructures such as Co and Fe nanowires at a Pt-surface step. Monte Carlo simulations have confirmed the existence of thermo-induced magnetism in antiferromagnet nanoparticles. We have developed an understanding of atomic displacement cascade evolution and the interaction between moving dislocations and nanometer-sized defects using MD simulations. An efficient global optimization strategy that allows use of additional available information to significantly reduce the computational complexity has been developed and is being applied to structural optimization of atomic clusters.

Program Impact: Our FLAPW calculations have supported alloy design of Ni-, Fe-, and Ti-based aluminides, and Mo-, Ti-based silicides, and have set the standard for first-principles calculations of ordered intermetallics. Our first-principles SCPW studies support the structural ceramics task and have provided a basic understanding of microstructure and mechanical properties of these materials. Many KKR-CPA codes used around the world had their genesis at ORNL. A version of the constrained local moment method developed at ORNL is being taken up by research groups in Europe. We are recognized leaders in applying parallel computing to materials science. We have provided insights and new methods to reduce the computational complexity of the global optimization problem related to nanocluster formation.

Interactions: Internal - six divisions and ten experimental and theory groups. External: six national laboratories, eight U.S. and seven foreign universities, three major corporations and four international research institutes. Past and current CRADAs include: IBM, Honeywell, Motorola, and Nonvolatile Electronics, Inc.

Recognitions, Honors, and Awards (at least partly attributable to support under this FWP or subtask):
Selected: C. L. Fu: ISI 1000 Most Cited Physicists; 2002 TMS Champion H. Mathewson Medal. G. S. Painter: APS Fellow. G. M. Stocks: APS Fellow, Computerworld Smithsonian Laureate (2000), Gordon Bell Award (3). R. E. Stoller: Fellow, ASTM; ANS Fusion Energy Division 2004 Outstanding Achievement Award.

Personnel Commitments for FY2005:
G. M. Stocks (70%), C.-L. Fu (100%), G. S. Painter (100%), Y. N. Osetskiy (50%), R. E. Stoller (35%), V. A. Protopopescu (30%), J. C. Wells (20%), B. Radhakrishnan (20%), J. Barhen (15%), J. R. Morris (10%), W. A. Shelton (10%), Z. Feng (5%), Support Staff (45%), Postdoctoral Staff (215%)

Authorized Budget (BA) for FY03, FY04, FY05:
FY03 BA $1699k **FY04 BA** $2595k **FY05 BA** $2268

Laboratory Name: Oak Ridge National Laboratory
B&R Codes: KC 02 01 01 0

FWP: Microscopy and Microanalysis

FWP Number: ERKCM03

Program Scope: The Microscopy and Microanalysis task involves operation and development of the SHaRE User Program (www.ornl.gov/share), applications to materials science, and research collaborations in the areas of analytical transmission electron microscopy (TEM) and scanning electron microscopy (SEM), atom-probe field-ion microscopy (APFIM), and nanoindentation.

Major Program Achievements (FY2003 – FY2005): Developed transmission electron aberration-corrected microscope (TEAM) project in collaboration with BES microscopy efforts at four other institutions, including co-hosting a workshop to develop vision and community support and achieving CD-0 and CD-1; coordinated jumpstart activities and hosted workshop for Center for Nanophase Materials Sciences (CNMS) Nanoscale Imaging, Characterization, and Manipulation; installed low voltage microprobe (LVM) with microcalorimeter energy-dispersive X-ray (EDX) spectrometer; installed and commissioned local electrode atom probe (LEAP); installed and commissioned dual-beam focused ion beam (DB-FIB) instrument; hosted international workshop on atom probe tomography (APT); developed methods to quantify size, shape, and composition of nanometer-scale features characterized by small clusters of atoms, as determined by APT; developed new analytical methods for measuring residual stress by nanoindentation with spherical indenter, correlating indentation size effects for spherical and sharp indenters; developed combinatorial methods for mechanical properties characterization; developed and refined a variety of analytical electron microscopy (AEM) techniques, including energy-filtered TEM, axial electron channeling microanalysis (ALCHEMI), low-voltage energy dispersive analysis, spectrum imaging, and orientation imaging microscopy (OIM); numerous applications to materials science.

Program Impact (FY2003 – FY2005): Microscopy community endorsement and sponsor support of TEAM development project; new microcharacterization methods and instrumentation developed in AEM, APFIM, and nanoindentation; broad-based utilization of SHaRE User Program.

Interactions (FY2003 – FY2005): SHaRE Facility usage included: 37 U.S. universities; 30 companies; 9 DOE national laboratories; 4 non-DOE federal laboratories with funding from DOE-Fusion Energy Sciences, DOE-Advanced Scientific Computing, DOE-Fossil Energy, DOE-Energy Efficiency and Renewable Energy; NSF, NASA, DARPA; ORNL LDRD Program.

Recognitions, Honors and Awards (FY2003 – FY2005): Anderson: 2004 Program Chair, Microscopy and Microanalysis 2004; Chair, Oak Ridge Chapter of ASM, 2002-2003 (ASM Chapter of Excellence Award Winner); Editorial Board of *Microscopy Research and Technique*, ongoing. Bentley: Chair, Awards Committee of Microscopy Society of America (MSA), 2003; Editorial Board of *Microscopy and Analysis*, ongoing. Kenik: 2005 American Nuclear Society Materials Science and Technology Special Achievement Award. Miller: 2004 Microscopy Society of America (MSA) Cosslett Award; Co-Chair, Focused Interest Group on Atom Probe, MSA, ongoing. Pharr: University of Tennessee (UT) Moses E. and Mayme Brooks Distinguished Professor Award, 2004; UT Chancellor's Award for Research and Creative Achievement, 2004; UT Research Fellow Award, ISI Citation Classic (2000+), 2005; Associate Editor, *J. Am. Ceram. Soc.*, ongoing; Guest Editor, special issue on instrumented nanoindentation, *J. Mater. Res.*, 2004.

Personnel Commitments for FY2005:
I. M. Anderson (75%), J. Bentley (90%), E. A. Kenik (80%), M. K. Miller (40%), N. D. Evans (UT, 40%), G. M. Pharr (Joint with UT, 30%), D. C. Joy (ORNL-UT Distinguished Scientist, 20%), M. J. Lance (10%), J. T. Busby (5%), Other Scientific Staff (15%), Support Staff (130%), Postdoctoral Staff (175%)

Authorized Budget (BA) for FY2003, FY2004, and FY2005:
FY03 BA $2335k **FY04 BA** $2520k **FY05 BA** $2035k

Laboratory Name: Oak Ridge National Laboratory
B&R Code: KC 02 01 05 0 and KC 02 06 01 0

FWP: Science of Non-equilibrium Processing of Materials

FWP Number: ERKCM05

Program Scope: The program addresses material behavior during non-equilibrium processing, focusing on welding and thermo-mechanical processing. The fundamentals of solidification behavior, correlation of thermal history with phase stability, and mathematical modeling of microstructure development are examined. It also seeks to develop a fundamental understanding of materials behavior under non-equilibrium thermo-mechanical processing using coupled multi-length scale modeling of deformation, recrystallization, and grain growth. The program also addresses material flow and microstructure modeling of friction stir welding process.

Major Program Achievements (over duration of support): Integrated solidification theory with a new geometric model to predict microstructure development including stray grain formation in single crystal welds. Identified non-equilibrium solidification behavior during laser welding. Developed 3-D transient, free surface fluid flow model for predicting weld pool geometry. Characterized phase stability of austenitic stainless steels and its influence on impact and creep properties. Developed a coupled thermodynamic and kinetic model for inclusion formation. Identified phase evolution during solidification of steel welds using in-situ synchrotron radiation experiments. Identified austenite phase separation through in-situ synchrotron diffraction experiments. Developed artificial neural network models for prediction of ferrite number in stainless steels and weld pool geometries. Organized seven international conferences on Trends in Welding Research. Developed a multiscale framework for modeling the microstructure and texture evolution during thermo-mechanical processing of materials by combining deformation models with Monte Carlo/phase field modeling and molecular dynamics simulations. The simulations yielded fundamental understanding of the evolution of cube texture in hot worked aluminum alloys and the formation and growth of special texture components in particle-containing alloys. Developed fundamental understanding of abnormal grain growth in friction stir processed material using mesoscale simulations. Developed a modeling framework to investigate material flow and defect formation in friction stir welding. Potential tool material for friction stir welding of steels and high temperature alloys was developed.

Program Impact: Has advanced the science of non-equilibrium processing and has led to numerous industrial applications and new program development.

Interactions: Internal—Microscopy and Microanalysis Group, Diffraction and Thermo Physical Properties Group. External—Pennsylvania State University; Cambridge University, U.K.; Technical University of Graz, Austria; Tokyo University, Japan; National Institute for Materials Science, Japan; Argonne National Laboratory; Lawrence Livermore National Laboratory; interactions with universities and national laboratories via Computational Materials Science Network (CMSN) projects.

Recognitions, Honors and Awards (at least in some part attributable to support under this program):
S .A. David—Editor in Chief, *Science and Technology of Welding and Joining*; TMS Fellow and Fellow of ASM International and AWS; Champion H. Mathewson award (2002); Arata Prize (2002); McKay Helm award (2002); UT-Battelle Director's and Distinguished Engineer award (2003). J. M. Vitek—Fellow-ASM International and AWS; Editorial Board, *Science and Technology of Welding and Joining*; McKay Helm award (2001); S .S. Babu—Editorial Board, *Science and Technology of Welding and Joining*; McKay Helm award (2002); Warren F. Savage award (2002); Lidstone Medal award (2003). B. Radhakrishnan—Board of Review, *Welding Journal*.

Personnel Commitments for FY2005:
S .A. David (15%), J. M. Vitek (30%), S. S. Babu (15%), B. Radhakrishnan (20%), G. Sarma (5%), Z. Feng (5%), Support Staff (30%)

Authorized Budget (BA) for FY03, FY04, FY05:
FY03 BA $791k **FY04 BA** $891k **FY05 BA** $415k

Laboratory Name: Oak Ridge National Laboratory
B&R Code: KC 02 01 02 0

FWP: High Temperature Alloy Design

FWP Number: ERKCM06

Program Scope: This program focuses on understanding ordered intermetallics and advanced metallic alloys, with emphasis on the fundamental variables that affect phase stability, microstructure, and mechanical behavior at ambient and elevated temperatures. This understanding leads to the development of broad scientific principles for the design of next-generation advanced materials for structural and functional use. Phase stability, point defects, and magnetic properties are correlated with site occupation, atomic bonding, and the electronic structure of intermetallic and metallic alloys. The observed relationships between mechanical properties and microstructural features (controlled, as needed, by innovative processing techniques and characterized by state-of-the-art microanalytical tools) are used to model the deformation and fracture of structural alloys. Efforts are also devoted to the understanding of physical and mechanical properties of bulk amorphous alloys and nanophase materials.

Major Program Achievements (over duration of support): Discovered moisture-induced environmental embrittlement as the mechanism responsible for low tensile ductility and poor fracture resistance of many high-symmetry intermetallics. Understood the ductilizing effect of boron and developed scientific principles for dramatically improving the ductility of Ni_3Al alloys. Developed a new theory based on thermal vacancies to explain the yield strength anomaly in FeAl alloys. Proposed several dislocation mechanisms to explain deformation twinning in hcp materials and $D0_{19}$ intermetallics. Substantially reduced thermal expansion anisotropy and microcracking in Mo_5Si_3 by quantum mechanical alloy design. Identified magnetic interaction as a new mechanism responsible for unusual solid solution effects observed in NiAl. Derived a new expression to predict the glass forming ability of bulk metallic glasses and other noncrystalline systems.

Program Impact: This program has provided national and international leadership in the field of intermetallic alloys and bulk metallic glasses through highly cited scientific publication and conference organization. Three principal investigators, C. T. Liu, E. P. George, and J. A. Horton, have been identified by ISA as the world's most-cited authors in material science during the past 20 years. The discovery of moisture-induced embrittlement as an extrinsic mechanism provided new directions for the design of ductile intermetallic alloys. By successfully combining theoretical calculations and experimental studies, this program has demonstrated the potential of designing engineering materials using a quantum-mechanical alloy design approach. The recent discovery of magnetic interaction is expected to provide new insights to explain unusual solid solution effects in intermetallic and metallic alloys. The comprehensive expression derived for glass forming ability serves as a useful tool to design new bulk metallic glasses with superior properties. Broad scientific principles derived from this BES program help DOE's applied programs in the design of ductile and strong intermetallic and metallic alloys for engineering use.

Interactions: As conducted within a world-leading research group in intermetallics and bulk metallic glasses, this task keeps close contact with many universities (including Universities of Pennyslvania, Tennessee, and Virginia, Brown, Kyoto, Tohoku, Beijing Science & Tech., Ruhr, and Technical University, Chemnitz), other national laboratories, and domestic and international materials institutes (IMR and NIMS, Japan) that are active in intermetallics and metals research.

Recognitions, Honors and Awards: C. T. Liu: 2004 member of the National Academy of Engineering, 2002 World Technology Network Fellow, 2001 *Acta Metallurgica* Gold Medal Award, 1994 TMS Fellow, Editor of *Intermetallics*; E .P. George: 2000 Humboldt Award, 1999 ASM Fellow; J .A. Horton: 2002 ASM Fellow; Z. P. Lu: 2004 *Phys. Rev. Lett.* paper identified by APS as one of the top physics stories of 2004, 2002 *Acta Mater*. paper identified by ISI as fast-moving front paper.

Personnel Commitments for FY2005: C. T. Liu (50%), Z. P. Lu (70%), J. R. Morris (65%), J. H. Schneibel (50%), J. A. Horton (40%), E. P. George (5%), Support Staff (110%), Postdoctoral Staff (290%)

Authorized Budget (BA) for FY03, FY04, FY05:
FY03 BA $1264k **FY04 BA** $1353k **FY05 BA** $1275k

Laboratory Name: Oak Ridge National Laboratory
B&R Code: KC 02 01 02 0

FWP: Microstructural Design of Advanced Ceramics

FWP Number: ERKCM07

Program Scope: Theory and experiment combine to define (1) the relationships between the properties of ceramics and the critical length-scale structural characteristics and (2) how these can be tailored during processing to enhance properties. The fundamental design concepts incorporate different length-scale characteristics into theoretical and analytical models that are used to tailor the behavior (e.g., toughness, mechanical reliability, creep resistance) of ceramics. The results provide a quantitative picture of the mechanisms that enhance the mechanical behavior of monolithic ceramics, composites, multilayer systems and coatings.

Major Program Achievements: This project develops the basis for compositional, as well as microstructural, tailoring of the next generation of ceramics for energy applications. Silicon nitride ceramics serve as a model system where amorphous intergranular films, which are ubiquitous in ceramics, impact mechanical behavior, as well as microstructure evolution. Recent results defined both the segregation behavior of additive elements, used in sintering, and its role in grain growth anisotropy. Analysis of the viscosity of model oxynitride glasses provided insights as to how rare earths impact creep resistance. Initial characterization revealed that this is due, in part, to changes in the bonding within the amorphous network. Scanning transmission electron microscopy observations combined with theoretical studies showed that the degree of segregation and ordering at the intergranular phase interfaces associated with two grain junctions, as well as triple point pockets, were a function of the specific rare earth present. Separate studies show that debonding of the reinforcing grains, responsible for toughening, exhibited a similar dependence on the rare earth , thereby demonstrating the significance of compositional design.

Program Impact: Provided theoretical and experimental insights into the microscopic and atomic scale origins of the mechanical behavior of ceramics that have led, and will lead, to toughened ceramics and novel design concepts for tailoring the properties of the next generation ceramics. These concepts have now been extended to include the role of atomic-level, as well as microscopic, characteristics.

Interactions:
Internal–Metals and Ceramics Division: Theory Group; Condensed Matter Sciences Division: Electron Microscopy Group and Thin Film and Nanostructured Materials Physics Group.
External–University of Karlsruhe, University of Tokyo, Oxford University, University of Tennessee, DuPont Central Research Laboratory, Commissariat à l´Énergie Atomique-Saclay, Korean Institute of Machinery and Materials, National Tsing Hua University.

Recognitions, Honors and Awards:
Thirteen invited presentations from this work at international conferences since 2003.
P. F. Becher: member of World Academy of Ceramics; Fellow, American Ceramic Society, member of National Materials Advisory Board (National Research Council, National Academies); Highly Cited Researcher in Materials Science, ISI Web of Knowledge; Alexander Von Humboldt Foundation Research Award for Senior Scientists (1991); American Ceramic Society: Purdy Publication Award (1988), Sosman Lecturer (1990), Society President, Associate Editor of Journal.
C. H. Hsueh: Fellow of the World Innovation Foundation; Fellow, American Ceramic Society; Highly Cited Researcher in Materials Science, ISI Web of Knowledge; Associate Editor, *Journal of the American Ceramic Society*; member editorial board of *Composite Engineering*.
M. J. Lance: ORNL Wigner Fellow (1998).

Personnel Commitments for FY2005:
P. F. Becher (75%), Chun-Hway Hsueh (80%), M. J. Lance (10%), Other Scientific Staff (10%), Support Staff (90%)

Authorized Budget (BA):
FY03 BA $1023k **FY04 BA** $1243k **FY05 BA** $1001k

Laboratory Name: Oak Ridge National Laboratory
B&R Code: KC 02 01 03 0

FWP: Domain Structure and Dynamics in Epitaxial Oxides

FWP Number: ERKCM29

Program Scope: From its inception, the broad scope of our research in thin-film oxides has been the dielectric physics of cooperative phenomena in oxide heterostructures on silicon, with the particular goal of understanding the fundamental length scales that control phase stability. Specifically we are approaching this goal via studies of field effect phenomena in crystalline oxides and studies of dielectric/optical properties in direct-gap chalcogenides. We are now expanding our program around our discovery of a whole class of strain-stabilized photovoltaic, sulfur-based chalcogenides that have direct gap electronic transitions and tunable band gaps. Heteroepitaxy of these compounds on the plentifully available cubic silicon surface will give us the much-sought-for double p-n junction photovoltaic structure that is required for dramatic improvements in solar cell efficiency. From these new chalcogenides, we can select structures and compositions in a double p-n junction device that will cover the complete solar spectrum with the possibility of achieving 40-60% efficiency in a semiconductor-based solar cell.

Major Program Achievements (over duration of support): Pioneered the field of dielectric physics based on crystalline oxides on semiconductors (COS). Demonstrated ferroelectric polarization reversal in a perfectly commensurate thin-film of $BaTiO_3$ on germanium enabling a two-logic transistor state that offers enormous potential for energy savings in a myriad of electronic sensors and devices. Developed a unifying reformulation of the classic Schottky Barrier Problem as it relates to dielectrics on semiconductors. Published our seminal findings in 1998 (*Phys Rev Lett.*). Since that paper, we have followed with several insightful publications, notably two in *Science*, in which the generalities of the physical and electrical structure for these COS systems and the Schottky Barrier work are presented .

Program Impact: Reformulation of the Schottky Barrier Problem is leading to an entirely new view of interface electrodynamics and interface phase thermodynamics that has broad implications in semiconductor/dielectric physics. These epitaxial oxides offer a unique opportunity to investigate the physics of Schottky barrier formation and charge transfer at the semiconductor-oxide interface, a problem that has accompanied us unyieldingly for over sixty years. This is apparent from focused symposia at U.S. and European scientific society meetings (at least two every year for the last five years) as well as commercial and DoD sector interest in technology applications, and our field-leading citation rate. Publications on this work are highly cited and are providing a substantial framework for both fundamental and applied research as these new materials are being developed.

Interactions: Collaboration with ORNL's (Malcolm Stocks) and NCSU's (Marco Buongiorno Nardelli) theory task is developing the electronic structure characteristics for several oxide/semiconductor systems. Collaborative research is being established with Prof. Kumar Das at Tuskegee and Prof. Alex Demkov at the Universtiy of Texas. A Penn State Ph.D. candidate (Curtis Billman) has finished his thesis work at ORNL on BaSrO and strain effects on silicon. A new student (Marton Zsolt) is beginning his Ph.D. work in collaboration with Prof. Egami at the University of Tennessee.

Recognitions, Honors and Awards (at least in some part attributable to support under this program):
Rodney McKee: Fellow of the American Physical Society, November 2003; International Advisory Committee, European Materials Research Society, Strasbourg Meeting, June 2003; Adjunct Professor at Penn State. McKee, Fred Walker, and Marco Nardelli presented 22 invited talks in major U.S. and European scientific societies (APS, MRS, TMS, ISIF, EMRS, and EPS) in the last 3 years. 20 U.S. and foreign patents and licensing arrangements (since 1998) to exploit a commercial transition of BES fundamental research to industry.

Personnel Commitments for FY2005:
R .A. McKee (65%), F. J. Walker, UT (65%)

Authorized Budget (BA) for FY05, FY06, FY07:
FY03 BA $396k **FY04 BA** $393k **FY05 BA** $377k

Laboratory Name: Oak Ridge National Laboratory
B&R Code: KC 02 06 02 0

FWP: Design and Synthesis of Nanomaterials

FWP Number: ERKCM38

Program Scope: This research addresses the controlled synthesis and directed assembly of nanoscale materials. The focus is on increasing the self-organization of nanophase material systems by enhancing and exploiting the interactions (e.g. between catalyst material and nanostructure or catalyst material and substrate); and on the controlled co-synthesis of magnetic nanoparticles that served as the growth catalyst and provide functionality. These materials exhibit emergent properties at the microscale and beyond size regime that are driven by the control of the material composition at the nanoscale. Theory, modeling, and simulation are an integral component of the synthesis effort. Phenomenological theory is used to determine the emergence of nanofiber structure and nanoparticle shape from basic kinematic principles. First principles quantum mechanical approaches are used to study order-disorder phenomena and the magnetic properties of nanoparticles relevant to the synthesis component.

Major Program Achievements (over duration of support): We have demonstrated the controlled synthesis of highly uniform silicon nanocones using a plasma enhanced chemical vapor deposition process and a copper catalyst material. We have also demonstrated the control of carbon nanofiber structure by manipulating the crystal orientation of catalyst thin films. In addition, following our phenomenological theory, we have demonstrated controlled nanofiber structure by utilizing the link between structure and growth rate. Self-assembled arrays of carbon nanofibers that mimic biological cell or membrane structures have been produced. In our theory efforts, first-principles electronic structure calculations produced insight into the elemental energetics and rate processes of the catalytic growth of carbon nanostructures on transition-metal catalysts.

Homogeneous nanostructures with particle-size distribution in a fairly narrow range of 5 to 10 nm were reported to form directly from casting the multicomponent alloy of $Zr_{60}Al_{15}Ni_{10}Co_{15}$. By careful analysis of microstructural features, we showed that the nanophased structures were produced through double eutectic decomposition reactions at relatively low temperatures.

We have performed proof-of-principle calculation of a realistic model of a ~5 nm nanoparticle of Fe that demonstrates the feasibility of direct quantum simulation of nanoparticle properties.

Program Impact: Our work with catalytically grown nanostructures demonstrates a degree of controlled synthesis and directed assembly that is already having an impact in areas such as the delivery of materials (e.g. genes, proteins, and therapeutic agents) to living cells, biomimetic structures, and field emission devices. This work addresses the fundamental nature and control of the catalytic growth process, which is still unclear in many cases, even for the simplest growth techniques. The methods developed under the theory component will be of quite general use for first-principles simulations of nanoparticle properties.

Interactions: University of California Santa Barbara: Biomolecular Science & Engineering Program (D. Morse); Brown University: Division of Engineering (K. S. Kumar); IBM Zurich Research Laboratory, ORNL-IBM CRADA (W. Andreoni and A. Curioni); University of Tennessee (P. K. Liaw, T. G. Nieh, and P. Rack); Pittsburgh Supercomputer Center (Y. Wang).

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask): M. L. Simpson was one of a small group invited to participate in National Academies Keck Future Initiative Workshop on "Designing Nanostructures at the Interface between Biomedical and Physical Systems."

Personnel Commitments for FY2005:
M. L. Simpson (10%), J. C. Wells (20%), T. G. Thundat (10%), Other Scientific Staff (5%), Postdoctoral Staff (170%)

Authorized Budget (BA) for FY03, FY04, FY05:
FY03 BA $280k **FY04 BA** $535k **FY05 BA** $483k

Laboratory Name: Oak Ridge National Laboratory
B&R Code: KC 02 01 03 0

FWP: Atomistic Study of Bulk Metallic Glasses

FWP Number: ERKCM40

Program Scope:
The recent development of bulk metallic glasses (BMG) has drastically improved the prospect of application of metallic glasses as a structural material. However, the science of metallic glasses, in particular at the atomistic level, is only in its infancy. The purpose of this project is to develop novel theoretical and experimental approaches to study the atomic level phenomena in metallic glasses. In particular, we will study glass transition, liquid viscosity, glass formation and mechanical deformation of BMG and aim to achieve an understanding of the mechanisms of BMG formation and deformation at an atomistic level. Our goal is to establish general principles that could guide the effort for further alloy development, including improvement of ductility. This year, this program absorbed ERKCM35 to strengthen our research on the atomistic mechanism of plastic deformation and atomic transport in metallic glasses.

Major Program Achievements (over duration of support): (New Program initiated in FY04; Funding arrived 9/04)
We have substantially extended our theory of topological fluctuations and have succeeded, for the first time, in deriving the analytical expressions for the glass transition temperature and the liquid fragility that agree exceptionally well with the experimental data, using only the microscopic variables (atomic volume, bulk and shear moduli and a critical strain). We view this as a major success, and as an indicator that our program is headed in the right direction. The key to this development was recognition of the importance of Poisson's ratio as a critical parameter. We developed a many-body potential with varying Poisson's ratio and used it in our molecular dynamics simulation. We have applied the theoretical techniques developed for ERKCM35, and formulated a model of collective atomic transport in viscous media. We also developed a model to account for chemical short-range order, which is usually not achievable by simulation due to the shortness of the physical time scale of simulation compared to the laboratory time scale, and proved it with TEM observation.

Program Impact: Our theory of glass transition and liquid fragility will impact not only bulk metallic glasses but covalent and molecular glasses as well. At present, the mode-coupling theory is the most widely used one in liquids. However, it is a phenomenological theory with up to seven fitting parameters. Our theory will provide the atomistic bases for the mode-coupling theory with the potential to impact a wide range of fields from engineering, physics, chemistry, medicine, and biology.

Interactions:
Internal – Computing and Computational Sciences, Computer Science and Mathematics Division, Condensed Matter Sciences Division, X-Ray Research and Applications Group, High Temperature Materials Laboratory, High Flux Isotope Reactor, Spallation Neutron Source.
External – Los Alamos National Laboratory, Ames Laboratory, California Institute of Technology, and the University of Virginia.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask): Six invited conference presentations on this subject in one year.

Personnel Commitments for FY2005:
T. Egami (ORNL-UT Distinguished Scientist, 50%), W. Dmowski (UT, 50%), Y. Y. Braiman (40%), V. A. Protopopescu (30%), J. R. Morris (15%), J. Barhen (15%), D. M. Nicholson (10%), G. M. Pharr (Joint with UT, 10%), Support Staff (5%), Postdoctoral Staff (250%)

Authorized Budget (BA) for FY03, FY04, FY05:
FY03 BA $ 0 **FY04 BA** $420k **FY05 BA** $955k

Laboratory Name: Oak Ridge National Laboratory
B&R Code: KC 02 02 03 0

FWP: Integrated Multiscale Modeling of Molecular Computing Devices

FWP Number: ERKCM41

Program Scope: Self-assembled molecular electronics (ME) systems composed of many single-molecule devices are conceived as the most promising path to future computers with ultra-dense, ultra-fast, molecular-sized components, and as the likely candidate to continue Moore's law beyond silicon technology. However, there exist formidable barriers to their practical implementation. Experiments in ME are both difficult and very expensive. We are developing a comprehensive theoretical and computational framework, especially for the prediction of electron transport in single molecules in their real environment (i.e., in a single-molecule experiment or at a system level in a working device). Significant theoretical and mathematical issues must be resolved to make such modeling capability a reality. In order to address this goal, this proposal brings together a team of experts to address process, device and circuit modeling of molecular electronics and the underlying mathematics in a comprehensive and integrated fashion across time and length scales.

Major Program Achievements (over duration of support): With the materials funding stream of this multi-disciplinary and multi-institution project, ORNL has been focusing upon theory and code for quantum electron transport in molecular and nanoscale systems. The non-orthogonal orbital transport code developed for this project is now fully functional. It demonstrates excellent performance on several architectures, including the Cray X1. We completed the interfacing with quantum mechanics via the NWChem code and with an optimally localized orbital code in collaboration with Prof. Bernholc's team from North Carolina State University.

The use of NWchem for transport calculations was illustrated on a system containing up to 6000 basis functions in the study of quantum transport properties of amphoterically doped carbon nanotubes; paper published in *J. Chem. Phys.*, 2005. Calculations of non-equilibrium transport properties (I-V curves) using optimally localized numerical orbitals led to another paper published in *Phys. Rev. Lett*., 2005.

A sustained effort towards benchmarking our methods with other published results was made possible and strengthened via a collaboration with the group of Prof. Hideo Sekino at the Technical University of Toyohashi, Japan, where a graduate student uses our code routinely to reproduce and comment on published works. We implemented the formal correspondence between Green function and scattering approaches in order to get more insights into the understanding of quantum effects (such as interference and other non-intuitive results) in transport-intrinsic behavior of some nano-scale systems and devices.

Using large-scale electronic structure calculations, we were able to develop a self-consistent description of the electronic processes taking place during the particular experimental situation of "Scanning Gate Microscopy;" the work was published in *Phys. Rev. Lett.* in December 2004.

Program Impact: Our new theoretical and computational tools are enabling more rigorous, complete and realistic modeling of molecular electronic devices and are already beginning to answer both fundamental and experimental questions. These codes will be widely available, including distribution as part of NWChem.

Interactions: Center for Nanoscale Materials (ANL) and Center for Nanophase Materials Sciences (ORNL); North Carolina State University; Technical University of Toyohashi.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
None

Personnel Commitments for FY2005:
V. Meunier (35%), X. G. Zhang (15%), Postdoctoral Staff (130%)

Authorized Budget (BA) for FY03, FY04, FY05:
FY03 BA $100k **FY04 BA** $194k **FY05 BA** $180k

Laboratory Name: Oak Ridge National Laboratory
B&R Code: KC 02 01 02 0

FWP: Self Assembly of Stable Nanoclusters in Metallic Matrices

FWP Number: ERKCM42

Program Scope: The goal of this program is to conduct basic research on the understanding of the formation mechanism, thermal stability, and hardening mechanism of extremely stable Ti-, Y-, and O-enriched nanoclusters (2-5 nm in diameter) observed in a ferritic alloy fabricated by mechanical alloying. Nanophase materials are known to be metastable in nature; consequently, these materials in bulk forms are usable only at relatively low temperatures because of coarsening processes that occur rapidly at elevated temperatures. The study of the scientific issues of these stable nanoclusters will possibly lead to identifying an interesting material state that is capable of extending the useful temperature range of nanophase materials from ambient to elevated temperatures. Initial study will focus on the ferritic alloy, with the intention to extend our study to include other metallic systems containing stable nanoclusters. This research is composed of two major tasks: (1) theoretical and experimental studies of the formation mechanism and thermal stability of stable nanoclusters in ferritic alloys and other metallic systems, and (2) experiment and modeling of hardening mechanisms of stable nanoclusters at ambient and elevated temperatures.

Major Program Achievements (over duration of support): (New program initiated in August, 2004). Atomic-scale characterization has established that these nanoparticles have a high degree of thermal stability even at temperatures close to 1400ºC. Atom probe tomography results for the as-milled powder have established that these nanoclusters form during the post-mill heat treatment. The time and temperature of the heat treatment are therefore the critical parameters for optimizing the size and number density of the nanoclusters and, consequently, determining the mechanical properties and the stability of the alloy. First-principles calculations carried out to understand the high oxygen concentration in the clusters suggest that stable bonding between oxygen and vacancies is necessary. In fact, the oxygen solubility in bcc-Fe can be as high as the concentration of pre-existing vacancies and reach a supersaturated state, if high vacancy defects can be created through non-equilibrium processes. The first-principles results also predict that vacancies play an indispensable role in enhancing the oxygen/cluster binding energy in the presence of Ti. This strong oxygen-vacancy binding makes stabilization of coherent nanoclusters in the Fe lattice feasible. The first atomic resolution scanning transmission electron microscopy (STEM) images of these materials have been obtained and show the Fe matrix contains clusters with diameters ranging from 2 to 5 nm and an average spacing of ~12 nm. The initial study of hardening behavior by TEM indicates that these clusters are profound barriers to dislocation movement, even at 1100°C.

Program Impact: The existence of nanoclusters that are thermodynamically stable at elevated temperatures is a truly intriguing issue in the materials community because of both the scientific implications of such a phenomenon and the potential applications. By successfully combining theoretical calculations and experimental studies, this project is expected to provide new understanding of the existence of nanoclusters that are thermodynamically stable at high temperatures. The scientific principles developed with this BES program are expected to have broad applicability in the synthesis of next-generation nanostructured materials with high temperature capability for engineering applications.

Interactions: Center for Nanophase Materials Sciences; Spallation Neutron Source; Groups in the Metals and Ceramics Division; Berlin Neutron Scattering Center, Hahn-Meitner-Institute, Berlin; Intense Pulse Neutron Source, ANL; Ohio State University; University of Tennessee; Washington University; Materials Science and Engineering Department, National Taiwan Ocean University.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
C.T. Liu: Member of National Academy of Engineering, 2004. M. K. Miller: 2004 MSA Cosslett Award; Co-Chair, Focused Interest Group on Atom Probe, MSA. C. L. Fu: ISI 1000 Most Cited Physicists

Personnel Commitments for FY2005: C. T. Liu (25%), M. K. Miller (15%), M. F. Chisholm (10%), Z. P. Lu (10%), D. T. Hoelzer (5%), M. J. Mills (Ohio State University, 15%), Support Staff 10%

Authorized Budget (BA) for FY03, FY04, FY05:
FY03 BA $0 **FY04 BA** $390 **FY05 BA** $374

Laboratory Name: Oak Ridge National Laboratory
B&R Code: KC 02 01 01 0

FWP: Atomistic Mechanisms of Metal-Assisted Hydrogen Storage in Nanostructured Carbon

FWP Number: ERKCM43

Program Scope: Development of a broad science foundation to identify and understand the atomistic mechanisms of metal-assisted hydrogen storage in nanostructured carbons. The research plan is organized on three interactive levels: (1) First-principle computations for simulation of hydrogen interactions with graphite-like structures and prediction of optimal material structures and properties; (2) Synthesis of appropriately modified metal-doped pitch precursors and preparation of activated carbon fibers as guided by the theoretical calculations; and (3) In-depth examination of the nanostructures of the carbon substrate and metal catalyst particles, and correlation of these structures with the hydrogen storage characteristics of the fibers.

Major Program Achievements (over duration of support): This program was funded in August, 2005.
Performed initial synthesis activities: Melt spun and stabilized control (pure) carbon fibers; prepared pitch precursor containing 1 wt% palladium.

Completed preliminary in-situ X-ray diffraction analysis of Pd-containing carbon fibers in hydrogen atmosphere at 1 bar.

Initiated grand canonical Monte Carlo simulation of hydrogen adsorption/desorption in graphite lattice.

Program Impact:
This project addresses long-term (2015) fundamental research needs in the area of design, modeling, fabrication, and characterization, at the nanoscale level and with atomic precision, of novel materials for hydrogen energy-related applications. This research will provide a sound understanding of the fundamental factors that influence hydrogen sorption on carbon materials and how they can be manipulated to attain the on-board storage targets for the FreedomCAR Program.

Interactions:
Significant collaboration with the Center for Advanced Engineering Fibers and Films, Clemson University; Involved with the IEA Hydrogen Implementing Agreement; Task 17: Solid and Liquid State Hydrogen Storage Materials, which includes: National Renewable Energy Laboratory, Savannah River National Laboratory, University of Québec (à Trois-Rivières-Canada), University of Nottingham (UK), Institute of Carbochemistry CSIC (Spain), and McGill University

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
Nidia Gallego, Member Advisory Committee – International Partnership for the Hydrogen Economy (IPHE) International Hydrogen Storage Technology Conference, 2005
Dan Edie, Member of Clemson University Steering Committee on Energy Research and Solutions

Personnel Commitments for FY2005:
N. C. Gallego (5%), Other Scientific Staff (5%)

Authorized Budget (BA) for FY03, FY04, FY05:
FY03 BA $0 **FY04 BA $0** **FY05 BA** $450k

Laboratory Name: Oak Ridge National Laboratory
B&R Code: KC 02 03 01 0

FWP and possible subtask under FWP: Materials for Catalysts

FWP Number: ERKCS05

Program Scope: Explore the synthesis, near surface properties, and chemical activity of materials for heterogeneous catalysis. Elucidate a 3-dimensional picture of the catalyst and support material including the defect composition and mobility, the space charge segregation, and the atomic structure at the support-catalysts interface. Synthesize model materials primarily by vapor deposition processes and characterize the catalytic activity with simple, but relevant reactions of small molecules. Materials and samples suitable for examination by aberration corrected electron microscopy, in coordination with the Electron Microscopy of Materials FWP, are emphasized.

Major Program Achievements (over duration of support):
Catalyst particles have been vapor deposited onto a tumbling, high-surface-area powder support. This novel process offers a number of practical and scientific advantages compared to the commonly used solution synthesis techniques. In particular, vapor deposition eliminates all sources of contamination associated with chemical precursors and greatly expands the selection of compositions for both the particle and support materials. Gold nanoparticles have been deposited onto a variety of substrate materials, including γ-alumina, fumed silica, activated and graphitic carbons, and titania. The particle size, catalytic activity, and thermal stability of the particles on different support materials have been correlated with potential energy calculations for gold atom addition to the surface. For some support materials, high-resolution *Z*-contract electron microscopy has identified dispersed single atoms of gold, in addition to the nanometer-sized gold clusters.

High specific surface area catalysts are also formed by co-deposition of both the support and catalyst phases using oblique-angle sputter deposition. With this technique, the composition of the support can be tuned as well as that of the catalyst particle. In addition, films have been deposited directly onto electrodes for characterization of electrical and electrochemical properties. Electrical studies of thin-film anatase+gold samples are beginning to clarify much of the confusing reports found in the literature where catalytic activity depends strongly on the pre-reaction conditioning.

New techniques are being developed for the characterization of the catalyst activity for gas reactions. Primary goals are increased sensitivity to facilitate characterization of very small area samples, and integrated techniques permitting physical characterization under reactive conditions. Using a batch reactor and infrared gas phase measurements, turn-over-frequencies and reaction kinetics have been probed accurately for very small samples. In the future, this will be combined with microbalance and electrical characterizations.

Program impact:
Provide a different perspective on the important field of catalysis where inorganic materials serve as both catalysts and active support materials. Our expertise in ceramic thin-film synthesis, defect properties, ionic and electronic conduction and electrochemical systems has been redirected to investigate materials of interest for catalyzed gas and liquid reactions and electrochemically promoted catalysis.

Interactions:
Battelle Columbus (J. Sayer)
Vanderbilt University (S. Rashkeev)
University of Milan, Dipartimento Chim Inorgan Met Organ & Analit (L. Prati)
University of Tennessee, Department of Chemistry (C. Barnes)
Department of Materials Science at MIT, Ceramics (Y. M. Chiang)
Department of Physics at University of South Florida (H. Srikanth, R. Hajndl, N. Frey)
Dow Chemical Corporation, Midland, MI (S. Babinec, M. Somasi)
A123 Systems, Boston, MA (B. Riley)

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
National Federal Laboratory Consortium Award of Excellence in Technology Transfer, 2004

Personnel Commitments for FY 2005 to Nearest =/- 10%:
N. J. Dudney (Group Leader) 60%; G. Veith 80%

Authorized Budget (BA) for FY 03, FY 04, FY 05:
FY 03 BA $645K **FY 04 BA $**600K **FY 05 BA $**560K

Laboratory Name: Oak Ridge National Laboratory
B&R Code: KC 02 02 03 0

FWP and possible subtask under FWP: Theory of Condensed Matter

FWP Number: ERKCS08

Program Scope: Research condensed matter physics theory using a broad range of computational and analytic approaches. The work includes the development and extension of modern theories of condensed matter and computational methods as well as applications. Present work includes highly correlated materials, superconductivity; ferroelectrics, materials design, magnetism and magnetic materials, magnetotransport, neutron scattering, multiscale modeling, magnetic nanostructures, molecular electronics, and various aspects of grain boundaries, surfaces, and interfaces. The long term goals are (1) to support and guide experimental research at ORNL and elsewhere, especially neutron science, nanoscience and novel materials discovery and (2) to develop theoretical and computational approaches for designing novel functional materials and nanostructures.

Major Program Achievements: Prediction of a novel Goldstone phonon mode in frustrated pyrochlores, understanding of step flow growth on vicinal surfaces, development of theory of complexity and colossal responses in correlated materials, elucidation of the importance of charge transfer and competition for charge in stabilizing or destabilizing intermetallic hydrides, understanding of mechanisms for synthesizing lead free piezoelectrics, elucidating the role of strong correlations in cuprate photoemission spectra, calculations of excitation spectra in transition elements and comparison with inelastic X-ray scattering, understanding the roles of the various cations in determining the specific the ferroelectric orderings in perovskites, prediction of the possibility of ferromagnetic correlations in quantum dot arrays, finding a kinetic pathway for formation of Fe nanowires on Cu surfaces, analysis of thermodynamic consistency of the double exchange model and applications to magnetic semiconductors, computational studies of phase fluctuations in high-T_c superconductors, development of a truncated polynomial expansion Monte Carlo method for fermion systems coupled to classical fields, elucidation of the initial phases of Ti growth on diamond, calculation of the three dimensional magnetic interactions in Na_xCoO_2 and understanding of the c-axis coupling mechanism, understanding the origin of the unusual hydrogen content of Mg_3MnH_7.

Program Impact: 28 invited talks given at international meetings and an additional 23 at universities; organization of five international conferences, organization of an ITP program, organizers of APS focus sessions and MRS symposia. Publications in high profile journals: In calendar year 2005 so far (January 1–September 30), the group has 35 published papers, including 13 *Physical Review Letters*, 1 *Science* article, and 1 *Nature* article.

Interactions: Internal—Center for Computational Sciences, Computer Science and Mathematics Division, Metals and Ceramics Division, Neutron and X-Ray Scattering groups, Electron Microscopy Group, Low-Dimensional Physics Group; Center for Nanophase Materials Science, Superconductivity, Synthesis and Properties of Novel Materials, and Correlated Electron Materials Group – External U.S. Universities: Cincinnati, Clemson, Georgetown, Harvard, Oklahoma State, Stanford, Texas A&M, Vanderbilt, William and Mary, and Universities of California (Davis, Irvine, Los Angeles, Santa Barbara, San Diego), Florida, Minnesota, Tennessee, Texas (Austin and Arlington) and Wisconsin., External U.S. Other Laboratories: Geophysical Laboratory, Naval Research Laboratory, External Foreign Country Collaborations: top institutions in Argentina, Austria, China, Denmark, France, Germany, India, Italy, Japan, and Sweden.

Recognitions, Honors, and Awards:
Member of nominating committee for Division of Computational Physics of the APS (A. Moreo); AAAS Fellow (S. Pantelides); 5 APS fellows; Distinguished Scientist (E. Dagotto); members of several editorial boards.

Personnel Commitments for FY 2005 to Nearest =/- 10%:
A. G. Eguiluz (Joint Faculty Participant) (50%); D. J. Singh (100%); R. S. Fishman (100%); S.T. Pantelides (Distinguished Visiting Scientist) (10%); K. Varga (ORNL Postdoc) (50%); Z. Zhang (70%); E. Dagotto (50%); A. Moreo (60%)

Authorized Budget (BA) for FY 03, FY 04, FY 05:
FY 03 $1035K **FY 04** $1126K **FY 05** $1575K

Laboratory Name: Oak Ridge National Laboratory
B&R Code: KC 02 02 02 0

FWP and possible subtask under FWP: Electron Microscopy of Materials

FWP Number: ERKCS18

Program Scope: Aberration-corrected scanning transmission electron microscopes with sub-Ångstrom beams are used to image the atomic structure of interfaces and grain boundaries with single atom-sensitivity. Electron energy loss spectroscopy allows elemental identification of single atoms within their bulk environment and determination of local electronic structure. Data from microscopy is combined with first-principles theory to provide insights into key issues in materials science, condensed matter physics, chemical sciences and nanoscience, including interfaces and grain boundaries, ultra-dispersed catalysts, nanotubes, nanocrystals, quasicrystals, complex oxides, and superlattices.

Major Program Achievements: The world's smallest electron beam—0.06-nm diameter. The ORNL press release was picked up by CNN and put on their website, followed by MSNBC, USA Today, and over 100 other sites worldwide over the following week. An interview on National Public Radio aired 2004, and articles appeared in the New York Times, the San Francisco Chronicle and many other newspapers and many trade journals around the world. First spectroscopic identification of single atoms. First imaging and lattice location of surface atoms on a rough, insulating oxide surface. First direct imaging of the so-called "charge-ordered" stripes in a mixed-valence manganite. First imaging of single dopant atoms in a ceramic grain boundary. Identification of a new dislocation core structure in a complex material.

Program Impact: Results have been influential on the commercial development of transmission electron microscopes and have helped to establish the DOE Transmission Electron Aberration-corrected Microscope (TEAM) project. Results are increasingly coupled with first-principles theory, and the resulting synergy offers quantitative insights into the atomic origins of materials properties, critical not only for the nanoscience revolution but also for all fields in materials and condensed matter sciences. Papers accepted recently to *Science*, *Nature*, *Nature Materials*, and *Physical Review Letters*. Program is actively involved in educational outreach with visits from teachers and students at all levels.

Interactions:
Internal—Condensed Matter Sciences Division: Theory Group, Thin Film and Nanostructures Group, Correlated Electron Materials Group; Metals and Ceramics Division: Ceramic Science and Technology Group, Carbon Technology Group; Chemical Sciences Division: Surface Chemistry and Heterogeneous Catalysis Group.
External—Universities: Vanderbilt; North Carolina State; North Carolina A&T; Drexel; Northwestern; Dartmouth College; Tokyo, Japan; Melbourne, Australia; Madrid, Spain; Pohang, Korea, Seoul National, Korea. National Institutes: LBNL, ANL, BNL, FS-MRL (TEAM); Polish Institute of Physics, Warsaw, Poland; Chinese Academy of Sciences, Beijing, China; Industries: Nion, Pixon, Fischione.

Recognitions, Honors, and Awards:
Materials Research Society Medal, 1992, Institute of Physics Thomas J. Young Medal and Award, 2001, Fellow of the American Association for the Advancement of Science, 2004. Group members presented ~40 invited talks in the last 12 months.

Personnel Commitments for FY 2005 to Nearest =/- 10%:
S. J. Pennycook (Group Leader) 30%; M. F. Chisholm 20%; Y. Peng 33%

Authorized Budget (BA) for FY 03, FY 04, FY 05:
FY 03 $573K **FY 04** $755K **FY 05** $955K

Laboratory Name: Oak Ridge National Laboratory
B&R Code: KC 02 01 01 0

FWP: Atomistic Mechanisms in Interface Science—Direct Imaging and Theoretical Modeling

FWP Number: ERKCS30

Program Scope: Aberration-corrected scanning transmission electron microscopes with sub-Ångstrom beams are used to image the atomic structure of interfaces and grain boundaries with single atom-sensitivity. Electron energy loss spectroscopy allows elemental identification of single atoms within their bulk environment and determination of local electronic structure. Data from microscopy is combined with first-principles theory to provide insights into key issues in materials science, condensed matter physics, chemical sciences and nanoscience, including interfaces and grain boundaries, ultra-dispersed catalysts, nanotubes, nanocrystals, quasicrystals, complex oxides, and superlattices.

Major Program Achievements: The world's smallest electron beam—0.06-nm diameter. The ORNL press release was picked up by CNN and put on their website, followed by MSNBC, *USA Today*, and over 100 other sites worldwide over the following week. An interview on National Public Radio aired 2004, and articles appeared in the *New York Times*, the *San Francisco Chronicle*, and many other newspapers and many trade journals around the world. First spectroscopic identification of single atoms. First imaging and lattice location of surface atoms on a rough, insulating oxide surface. First direct imaging of the so-called "charge-ordered" stripes in a mixed-valence manganite. First imaging of single dopant atoms in a ceramic grain boundary. Identification of a new dislocation core structure in a complex material.

Program Impact: Results have been influential on the commercial development of transmission electron microscopes and have helped to establish the DOE Transmission Electron Aberration-corrected Microscope (TEAM) project. Results are increasingly coupled with first-principles theory, and the resulting synergy offers quantitative insights into the atomic origins of materials properties, critical not only for the nanoscience revolution but also for all fields in materials and condensed matter sciences. Papers accepted recently to *Science*, *Nature*, *Nature Materials*, and *Physical Review Letters*. Program is actively involved in educational outreach with visits from teachers and students at all levels.

Interactions:
Internal—Condensed Matter Sciences Division: Theory Group, Thin Film and Nanostructures Group, Correlated Electron Materials Group; Metals and Ceramics Division: Ceramic Science and Technology Group, Carbon Technology Group; Chemical Sciences Division: Surface Chemistry and Heterogeneous Catalysis Group.
External—Universities: Vanderbilt; North Carolina State; North Carolina A&T; Drexel; Northwestern; Dartmouth College; Tokyo, Japan; Melbourne, Australia; Madrid, Spain; Pohang, Korea; Seoul National, Korea. National Institutes: LBNL, ANL, BNL, FS-MRL (TEAM); Polish Institute of Physics, Warsaw, Poland; Chinese Academy of Sciences, Beijing, China; Industries: Nion, Pixon, Fischione.

Recognitions, Honors, and Awards:
S. J. Pennycook: Materials Research Society Medal, 1992; Institute of Physics Thomas J. Young Medal and Award, 2001; Fellow of the American Association for the Advancement of Science, 2004. Group members presented ~40 invited talks in the last 12 months.

Personnel Commitments for FY 2005:
S. J. Pennycook (5%), M. F. Chisholm (50%), M. Varela del Arco (30%), N. DeJonge (10%), Support Staff (140%), Postdoctoral Staff (160%)

Authorized Budget (BA) for FY03, FY04, FY05:
FY03 BA $599k **FY04 BA** $1045k **FY05 BA** $1003k

Laboratory Name: Oak Ridge National Laboratory
B&R Code: KC 02 02 02 0

FWP and possible subtask under FWP: Functional Nanomaterials: Growth Mechanisms and Properties

FWP Number: ERKCS72 (ERKCS04, ERKCS32, and ERKCS49 combined into ERKCS72 in FY 2005)

Program Scope: This program addresses the two central challenges of nanoscale science: First, to understand complex, self-organizing behavior and, second, to control growth mechanisms and direct the assembly of materials with enhanced or entirely new combinations of properties. The materials focus is on epitaxial heterostructures of complex metal oxides grown with atomic-layer control, and on carbon and other nano-tubes/fibers/wires/belts that exhibit effects of reduced and experimentally variable dimensionality, including ordered arrays. The program's strength is its integration of three key capabilities: advanced synthesis, detailed characterization (nanoscale to bulk), and modeling/simulation. For synthesis, emphasis is placed on energetic-beam methods—pulsed-laser deposition (PLD), laser vaporization, and plasma-enhanced CVD—and on time-resolved, in situ diagnostics of growth and kinetics. For ex situ characterization, scanning probes, electron microscopy, and electronic, magnetic, and transport measurements are used. Theory and experiment are highly integrated for understanding both growth and properties. Modeling/simulation is carried out with leading ORNL and external theorists. Microsecond time-resolved surface synchrotron x-ray diffraction (SSXRD) at the Advanced Photon Source is used with modeling to study surface evolution during PLD, in order to kinetically manipulate oxide growth. Effects of nanoscale structure, confinement, chemical attachment, and interlayer coupling on functional properties are studied, and key experimentally measured and calculated parameters are compared, to test and develop theoretical tools for materials-by-design.

Major Program Achievements (FY 2005): (1) First experimental verification of theoretically predicted polarization enhancements in artificial dielectric-ferroelectric superlattices, with properties surpassing those of the constituents. (2) Complete solution of the 2D Hubbard model for high-T_c superconducting cuprates with $T_c \sim 70$K. (3) Combined experimental-theoretical construction of a generic morphological phase diagram delineating conditions for persistent step-flow growth of oxide films. (4) Time-resolved SSXRD first observation and modeling of strong two-level-system layer filling during oxide PLD. (5) First in situ time-resolved reflectivity measurements of carbon nanotube CVD growth kinetics and development of a rate-equation model. (6) Growth and flash diffusivity measurements of millimeters-long vertically aligned (VA) carbon nanotube arrays with thermal diffusivities >0.8 cm^2/s and large thermal anisotropies (>70:1). (7) Molecular beam-controlled growth and modeling of dense VA single wall carbon nanotube (SWNT) arrays, decoupling surface and gas-phase reactions. (8) Simulations demonstrating non-diffusive spin waves exist in paramagnets, and predicting neutron scattering's use to discover precursors to magnetic ordering. (9) Atomic-resolution visualization of localized holes in manganite films.

Program Impact: Leaders internationally in the design and synthesis of artificial oxide heterostructures with enhanced properties, and in using time-resolved in situ diagnostics to understand nonequilibrium growth environments. Definitive exploration of TMO cooperative phenomena, and development and testing of theoretical models. Development of nano-structured materials for efficient energy use: multi-layered oxide-film fuel cells, CNT-based multifunctional structural materials, and efficient solid-state lighting. Deterministic growth of VA carbon nanofibers, enabling use by other programs for gene transfer, electrochemical probing of living cells, and electron field emission. High educational impact: well integrated program for grad student or postdoctoral research.

Interactions: *External*—Collaboration/subcontract on SWNT crystals with R. Smalley (Rice). 41 other collaborations with universities, including leading external theorists, grad students and postdocs. BES/DOE S&P and other collaborations on carbon-based materials with Argonne, Brookhaven, and Sandia NLs. Collaborations with 21 other U.S. and foreign national/industrial research labs. *Internal*—Oxide heterostructures synthesized with atomic-layer control are indispensable to test theory/modeling using leadership scientific computing facilities, and to exploit atomic-scale spectroscopy based on z-contrast scanning transmission electron microscopy.

Recognitions, Honors, and Awards (FY 2005, at least partially attributable to support under this FWP or subtask): 39 invited talks at national/international conferences/workshops; 26 invited colloquia and seminars; 2 invited reviews; Presidential Early Career Award; Scientific Director, *Center for Nanophase Materials Sciences*; co-leader, DOE Computational Materials Network; several ORNL research awards; 10 invention/patent disclosures and 3 U. S. patents issued; co-organizers of 12 international conferences (including APS, MRS, European-MRS, SPIE); 5 international program committees; supervision of 10 Ph.D. theses; service on Ph.D. exam committees.

Personnel Commitments for FY 2005 to Nearest =/- 10%: H. N. Lee, 90%; G. Eres, C. M. Rouleau, 80%; D. B. Geohegan, H. M. Christen, 50%; Z. Pan, 30%; A. A. Puretzky, J. Z. Tischler, 20%; G. E. Jellison, B. C. Larson, D. H. Lowndes, D. G. Mandrus, J. Shen, T. C. Schulthess, Z. Zhang, 10%; 3.1 postdocs/guest scientists; tech. 60%.

Authorized Budget (BA) for FY 03, FY 04, FY 05:
FY 03 $2,423K **FY 04** $2,350K **FY 05** $2,175K

Laboratory Name: Oak Ridge National Laboratory
B&R Code: KC 02 02 01 0

FWP and possible subtask under FWP: X-Ray Scattering and Microscopy

FWP Number: ERKCS73 (ERKCM02, ERKCS09, and ERKCS39 combined into FWP ERKCS73 in FY 2005)

Program Scope: Ultra-high brilliance x-rays from synchrotron beamlines at the Advanced Photon Source (APS) are exploited in connection with innovative instrumentation, advanced measurement techniques, and theory collaborations to conduct fundamental investigations of the atomic and electronic structure of materials and the impact of local structure and microstructure on materials properties. Novel x-ray focusing optics and three-dimensional (3D) submicron-resolution x-ray microdiffraction techniques are developed to probe materials microstructure and evolution on mesoscopic length scales (tenths of microns to hundreds of microns). Questions addressed include long-standing materials issues such as 3D grain-growth, fundamental aspects of deformation, and strain localization. Non-resonant inelastic x-ray scattering is used to study the dynamical electronic structure of strongly correlated electron materials, elastic diffuse scattering is used to probe short-range atomic structure in alloys, and Bragg and surface scattering is used to probe strain and phase in bulk materials and structure and epitaxy in thin-films. Advanced neutron optics and novel scattering techniques are developed to extend neutron applications to 3D measurements of local materials structure and to small sample sizes.

Major Program Achievements: Demonstrated polychromatic x-ray optics with less than 100 nm beam size, and polychromatic neutron optics that efficiently focus to less than 100 μm; developed a polychromatic microdiffraction beam line on UNICAT-II (Sector 34) at the APS; developed 3D x-ray structural microscopy for submicron-resolution measurements of crystal structure, orientation, and strain tensor distributions; performed the first micron-resolution, nondestructive, 3D measurements of thermal grain-growth and boundary motion; absolute, measurement of plastic deformation with submicron resolution over mesoscopic length scales using microindents; combined inelastic x-ray scattering with energy-resolved Wannier function analyses to identify new symmetry selection rules in transition metal monoxides; pioneered new methods to study fundamental properties of solid solution alloys.

Program Impact: This program has developed the only x-ray facility providing 3D crystal structure, orientation, and local elastic and plastic strain tensors with submicron resolution – a direct and previously missing link between the actual structure/evolution of materials and theory, simulations, and multiscale modeling. X-ray optics and polychromatic microbeam analyses developed in this program are being integrated into synchrotron microbeam facilities in Canada, Australia, and Italy. Absolute measurements of inelastic x-ray scattering for arbitrary materials provides the first absolute test of *ab initio* dynamical electronic response calculations for strongly correlated materials. Advanced nanoprobe optics will enable unique experimental characterization of individual nanoparticles. Polychromatic neutron focusing optics will increase neutron flux by two orders of magnitude for beams less than 100 microns and they will facilitate neutron measurements with 3D spatial resolution and in small sample volumes.

Interactions: U. Illinois MRL; NIST; APS, ALS, ESRF, Canadian, Australian, and Pohang (Korea) Synchrotron facilities; Sandia National Lab.; LANSCE, IPNS, and Chalk River; U. Tennessee; Florida State Univ.; U. Florida; Carnegie-Mellon; U. Western Ontario; U. Michigan; The Ohio State Univ.; U. Southern California; Mississippi State Univ.; Lehigh Univ.; State Univ. of New York; Stonybrook; Indian Institute of Science; Institute Metal Physics, Ukraine; Alcoa Technical Center; Northrup-Grumman; Ford Motor Company; General Motors; IBM; Industrial Whiskers Fundamental Task Force; NASA.

Recognitions, Honors, and Awards: 2005 Maslen Fellow, R&D 100 Award for "Differentially Deposited X-Ray Microfocusing Mirrors" (2000); 2 APS Fellows, ASM Fellow, Co-editor *Journal of Synchrotron Radiation*; Guest Editor, *MRS Bulletin* (March 2004); UT-Battelle Scientific Research by Team Award (2002); Chair, APS Beam Time Allocation Committee (2002–2005); APS User's Organization Steering Committee, (2003–2006); more than 30 invited talks (2003–2005).

Personnel Commitments for FY 2005 to Nearest =/- 10%: B. C. Larson (80%); G. E. Ice (75%); J. D. Budai (100%); J. Z. Tischler (80%); J. Pang (100%); E. Specht (65%); Guest Scientists: R. Barabash (100%), W. Yang (100%).

Authorized Budget (BA) for FY 03, FY 04, FY 05:
FY 03 $2,146K **FY 04** $2,150K **FY 05** $2,350K

Laboratory Name: Oak Ridge National Laboratory
B&R Code: KC 02 02 02 0

FWP and possible subtask under FWP: Materials by Design
FWP Number: ERKCS74 (In FY 2005, ERKCS06, ERKCS15, ERKCS52, and ERKCS53 were combined into ERKCS74.)
Program Scope: The focus of this program is science-driven synthesis and fabrication of new materials with novel properties and functionality. This is accomplished by a two-pronged approach involving (1) the development and growth of crystalline materials with innovative properties and (2) a "materials-by-design" approach using molecular beam epitaxy (MBE), laser MBE, and other novel growth processes to control properties with environment and dimensionality. One main theme of the research is to control and design materials that display complex, cooperative phenomena such as superconductivity, magnetism, metal-insulator transitions, ferroelectricity, optoelectricity, and optomagnetism. An essential component of this program is the development of advanced instrumentation and measurement techniques to characterize the functionality of these materials.
Major Program Achievements (over duration of support): The following bullets highlight this year's success. The first 11 are *Physical Review Letters* published this year.

- STM observation of a low temperature disordered phase of α-Pb/Ge(111), PRL **94**, 36105 (2005).
- A detailed STM study of the intertwined electronic and structural phase transitions in the In/Si(111) interface, PRL **95**, 046102 (2005).
- Report of a Goldstone-mode phonon dynamics in the pyrochlore $Cd_2Re_2O_7$, PRL **95**, 5503 (2005).
- The observation of non-Fermi liquid behavior in quasi-one-dimensional $Li_{0.9}Mo_6O_{17}$, PRL (accepted).
- Real-space observation of nanoscale inhomogeneities and fluctuations in a phase transition of a surface quasi-one-dimensional system: In/Si(111), PRL **95**, 116103 (2005).
- An optical study of interactions in a d-electron Kondo lattice with ferromagnetism, PRL **95**, 6401 (2005).
- Visualization of localized holes in manganite thin films with atomic resolution, PRL (accepted).
- Frozen low-spin interface in ultrathin Fe films on Cu(111), PRL **95**, 27201 (2005).
- Observation of multiple Bosonic mode coupling in electron self-energy of $(La_{2-x}Sr_x)CuO_4$, PRL **95**, 117001 (2005).
- The observation of a new magnetic anomaly below the ferromagnetic Curie temperature in $Yb_{14}MnSb_{11,}$ PRL (accepted).
- Observation of the Fermi surface evolution and Luttinger theorem in Na_xCoO_2: A systematic photoemission study, PRL **95**, 6401 (2005).

Other major achievements:

- Discovered a new mechanism for nanowire formation though ion irradiation, *Advanced Materials* (accepted).
- Identification the mechanism for magnetic polaron formation and percolation in dilute doped Mn_xGe_{1-x} magnetic semiconductors, APL **86**, 152507 (2005).
- Electromechnical imaging of biological systems with sub-10 nm resolution, APL **87**, 053901 (2005).
- Identified and quantified anomalously low flux creep rates in superconducting MgB_2 films, *Supercond. Sci. Technol.* **18**, 970 (2005).
- Demonstrated greatly enhanced flux pinning in YBCO films by controlled introduction of second phase Y_2O_3 nanoparticles as flux pinning centers, *Supercond. Sci. Technol.* **18**, 1502 (2005).

Program impact: This program has produced >89 papers, 1 patent, and >31 invited talks at national and international meetings.
Interactions: Extensive collaborations exist within ORNL. There are ~70 national and international collaborations leading to published papers and joint external proposals.
Recognitions, Honors, and Awards (at least partly attributable to support under this FWP or subtask):
J. Shen, 2005 ORNL Significant Event Award. **Maria Torija**, Leo Falicov Award presented at the 2004 American Vacuum Society symposium. **Hanno Weitering**, Joint Institute for Advanced Materials Chair of Excellence.
Personnel Commitments for FY 2005 to Nearest =/- 10%:
A. P. Baddorf (40%); L. A. Boatner (40%); C. Cantoni (80%); D. K. Christen (10%); S. Jesse (ORNL postdoc) (25%); R. Jin (90%); S. V. Kalinin (60%); A. P. Li (ORNL postdoc) (30%); J. Ma (UT research associate) (30%); D. G. Mandrus (90%); I. Paulauskas (UT graduate student) (100%); E. W. Plummer (Distinguished Scientist) (46%); J. O. Ramey (25%); B. Sales (90%); J. Shen (40%); J. Shin (UT graduate student) (100%); J. R. Thompson (10%); W. Tian (UT graduate student) (50%); H. H. Weitering (joint UT faculty) (30%); J. F. Wendelken (60%); H. Zhai (ORNL postdoc) (25%)
Authorized Budget (BA) for FY 03, FY 04, FY 05:
FY 03 $2575K **FY 04** $2858K **FY 05** $2855K